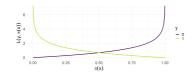
Introduction to Machine Learning

Optimal constant model for the empirical log loss risk (deep-dive)





Learning goals

- Derive the optimal constant model for the binary empirical log loss risk
- Derive the optimal constant model for the empirical multiclass log loss risk

BINARY LOG LOSS: EMP. RISK MINIMIZER

Given $n \in \mathbb{N}$ observations $y^{(1)}, \dots, y^{(n)} \in \mathcal{Y} = \{0, 1\}$ we want to determine the optimal constant model for the empirical log loss risk.

$$\underset{\theta \in (0,1)}{\arg \min} \, \mathcal{R}_{\text{emp}} = \underset{\theta \in (0,1)}{\arg \min} - \sum_{i=1}^{n} y^{(i)} \log(\theta) + (1 - y^{(i)}) \log(1 - \theta).$$



BINARY LOG LOSS: EMP. RISK MINIMIZER / 2

The minimizer can be found by setting the derivative to zero, i.e.,

$$\frac{d}{d\theta}\mathcal{R}_{\text{emp}} = -\sum_{i=1}^{n} \frac{y^{(i)}}{\theta} - \frac{1 - y^{(i)}}{1 - \theta} \stackrel{!}{=} 0$$

$$\iff -\sum_{i=1}^{n} y^{(i)} (1 - \theta) - \theta (1 - y^{(i)}) \stackrel{!}{=} 0$$

$$\iff -\sum_{i=1}^{n} \left(y^{(i)} - \theta \right) \stackrel{!}{=} 0$$

$$\Rightarrow \hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} y^{(i)} \in (0, 1) \checkmark \text{(assuming both labels occur)}.$$



MULTICLASS LOG LOSS: EMP. RISK MINIMIZER

Given $n \in \mathbb{N}$ observations $y^{(1)}, \dots, y^{(n)} \in \mathcal{Y} = \{1, \dots, g\}$ with $g \in \mathbb{N}_{>1}$ we want to determine the optimal constant model $\theta \in (0, 1)^g$ for the empirical log loss risk

$$\underset{\theta \in (0,1)^g}{\operatorname{arg\,min}} \, \mathcal{R}_{\mathsf{emp}} \quad = \quad \underset{\theta \in (0,1)^g}{\operatorname{arg\,min}} - \sum_{i=1}^n \sum_{j=1}^g \mathbb{1}_{\{y^{(i)} = j\}} \log(\theta_j)$$

$$\mathsf{s.t.} \quad \sum_{j=1}^g \theta_j = \mathsf{1}.$$

We can solve this constrained optimization problem by plugging the constraint into the risk (we could also use Lagrange multipliers), i.e., we replace θ_g (this is an arbitrary choice) such that $\theta_g = 1 - \sum_{j=1}^{g-1} \theta_j$.



MULTICLASS LOG LOSS: EMP. RISK MINIMIZER / 2

With this, we find the equivalent optimization problem

$$\begin{array}{ll} \mathop{\arg\min}_{\theta \in (0,1)^{g-1}} \mathcal{R}_{\text{emp}} & = & \mathop{\arg\min}_{\theta \in (0,1)^{g-1}} - \sum_{i=1}^{n} \sum_{j=1}^{g-1} \mathbbm{1}_{\{y^{(i)} = j\}} \log(\theta_j) \\ & & + \mathbbm{1}_{\{y^{(i)} = g\}} \log\left(1 - \sum_{j=1}^{g-1} \theta_j\right) \\ & \text{s.t.} & \sum_{j=1}^{g-1} \theta_j < 1. \end{array}$$

For $j \in \{1, \dots, g-1\}$, the *j*-th partial derivative of our objective

$$\frac{\partial}{\partial \theta_{j}} \mathcal{R}_{emp} = -\sum_{i=1}^{n} \mathbb{1}_{\{y^{(i)}=j\}} \frac{1}{\theta_{j}} - \mathbb{1}_{\{y^{(i)}=g\}} \frac{1}{1 - \sum_{j=1}^{g-1} \theta_{j}}$$
$$= -\frac{n_{j}}{\theta_{i}} + \frac{n_{g}}{\theta_{g}}$$

where n_k with $k \in \{1, ..., g\}$ is the number of label k in y and we assume that $n_k > 0$.



MULTICLASS LOG LOSS: EMP. RISK MINIMIZER / 3

For the minimizer, it must hold for $j \in \{1, \dots, g-1\}$ that

$$\frac{\partial}{\partial \theta_{j}} \mathcal{R}_{emp} \stackrel{!}{=} 0$$

$$\iff -n_{j}\theta_{g} + n_{g}\theta_{j} \stackrel{!}{=} 0$$

$$\Rightarrow \sum_{j=1}^{g-1} (-n_{j}\theta_{g} + n_{g}\theta_{j}) \stackrel{!}{=} 0$$

$$\iff -(n - n_{g})\theta_{g} + n_{g}(1 - \theta_{g}) \stackrel{!}{=} 0$$

$$\iff -n\theta_{g} + n_{g} \stackrel{!}{=} 0$$

$$\iff \hat{\theta}_{g} = \frac{n_{g}}{n} \qquad \in (0, 1) \checkmark$$

$$\Rightarrow \forall j \in \{1, \dots, g-1\} : \quad \hat{\theta}_{j} = \frac{\hat{\theta}_{g}n_{j}}{n_{g}} = \frac{n_{j}}{n} \qquad \in (0, 1) \checkmark$$

$$(\Rightarrow \sum_{j=1}^{g-1} \hat{\theta}_{j} = 1 - \hat{\theta}_{g} = 1 - \frac{n_{g}}{n} < 1\checkmark)$$



CONVEXITY

Finally, we check that we indeed found a minimizer by showing that \mathcal{R}_{emp} is convex for the multiclass case (binary is a special case of this):

The Hessian of $\mathcal{R}_{\mathsf{emp}}$

$$abla^2_{ heta}\mathcal{R}_{\mathsf{emp}} \;\; = \;\; egin{pmatrix} rac{ec{ heta}_1^2}{ heta_1^2} & 0 & \dots & 0 \ 0 & \ddots & \ddots & ec{ heta} \ dots & \ddots & \ddots & 0 \ 0 & \dots & 0 & rac{n_{g-1}}{ heta_g^2} \end{pmatrix}$$

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is positive definite since all its eigenvalues

$$\lambda_j = \frac{n_j}{\theta_j^2} > 0 \quad \forall j \in \{1, \dots, g-1\}.$$

From this, it follows that \mathcal{R}_{emp} is (strictly) convex.